

Operations with this Structure (NSC 77427):

Structure
Retrieval:Format:

Fields:

Retrieve

Cell Screens:

Yeast Screen

Format:

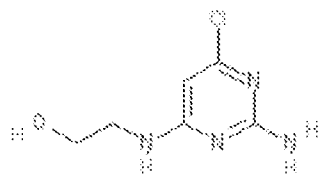
Retrieve

Visualization:

Format:

Display

Structure Data:



NSC Number: 77427

Date: 2011-09-21
05:38

File Record: 62076

CAS
Number: 2846-77-7Formula: C₆H₉ClN₄OWeight: 188.6163
gr/mol

Complexity: 136.7

Anti-HIV
Screening: No data
available

Druglikeness(std):

Is drug

logP(KOW): -0.82

Druglikeness(neg):

Is drug

logP(exp): No data

WDI Record:

No

logP(ACD): No data

H-Bond Acceptors:

5

Available on
DTP Plates: Yes

H-Bond Donors:

3

Rotatable Bonds: (CACTVS)

3

WLN: No data

Stereochemistry Potential

No

R/S atoms and E/Z bonds

Yeast
Screen
Level: 1

Catalyst Conformers:

21

(0 if Catalyst could not handle structure)

Matched
Conformer: None[Transfer to Java Editor](#)

Composition:

C 38.21% H 4.81% N 29.70% Cl 18.80% O 8.48%

SMILES:

NC1=NC(=CC(=N1)Cl)NCCO

Name:

2-((2-amino-6-chloro-4-pyrimidinyl)amino)ethanol (ACD/Name 4.0)

Commercial Availability:

No

Commercial Database Keys:

None

Available Screening Data:

Yeast

Anti-HIV Screening:

No data (EC₅₀/IC₅₀) available.

Cancer Screening Summary:

No data (GI₅₀/TGI/LC₅₀) available.

PASS Predictions:

Predicted Activity

Acetylcholine agonist
 Acetylcholine muscarinic agonist
 Acetylcholine nicotinic agonist
 Adenosine A2a receptor agonist
 Adenosine A2a receptor antagonist
 Adenosine A2 receptor agonist
 Adenosine A2 receptor antagonist
 Adenosine A3 receptor antagonist
 Alcohol dehydrogenase inhibitor
 Antibiotic Trimethoprim-like
 Antihypercholesterolemic
 Antiinfective (HIV)
 Antimalarial
 Antimetabolite
 Antineoplastic
 Antiobesity

p(active)	p(inactive)
0.199	0.085
0.123	0.093
0.181	0.136
0.195	0.025
0.072	0.032
0.038	0.016
0.068	0.041
0.286	0.210
0.261	0.199
0.127	0.006
0.314	0.096
0.505	0.030
0.247	0.061
0.267	0.016
0.317	0.135
0.223	0.134

Antiprotozoal	0.338	0.053
Antismoking	0.569	0.012
Antitrichomonal	0.270	0.071
Antitrypanosomal	0.333	0.036
Antiviral	0.685	0.009
Antiviral (HIV)	0.433	0.016
Antiviral (influenza)	0.123	0.001
Atherosclerosis treatment	0.581	0.085
Benzodiazepine agonist partial	0.213	0.042
Cannabinoid receptor agonist	0.254	0.037
Carcinogenic	0.219	0.081
Cholinergic agonist	0.290	0.200
Cytostatic	0.391	0.048
Dihydrofolate reductase inhibitor	0.147	0.006
Diuretic	0.237	0.129
Erythropoietin	0.490	0.020
Glycinamide ribonucleotide formyltransferase inhibitor	0.052	0.014
Growth stimulant	0.176	0.128
HDL-cholesterol increasing	0.323	0.110
Hematopoietic inhibitor	0.493	0.011
3 Hydroxyanthranilate oxygenase inhibitor	0.296	0.148
5 Hydroxytryptamine 3 agonist	0.614	0.008
Hypoglycemic	0.169	0.129
Interferon inducer	0.277	0.051
Interleukin 6 antagonist	0.377	0.221
Interleukin 8 antagonist	0.166	0.080
Multiple sclerosis treatment	0.584	0.064
Neuropeptide antagonist	0.313	0.100
Neuropeptide Y antagonist	0.313	0.100
NMDA receptor glycine site agonist	0.287	0.201
Nucleotide metabolism regulator	0.394	0.147
O6-alkylguanine-DNA alkyltransferase inhibitor	0.117	0.007
Protein kinase C inhibitor	0.274	0.042
Purine nucleoside phosphorylase inhibitor	0.068	0.019
Purinerbic P2 antagonist	0.130	0.037
Purinerbic P2T antagonist	0.091	0.030
Purinerbic receptor antagonist	0.130	0.037
Radiosensitizer	0.243	0.155
Reverse transcriptase inhibitor	0.488	0.007
Sclerosant	0.232	0.203
Septic shock treatment	0.369	0.109
Sodium channel blocker	0.464	0.029
Thymidylate synthase inhibitor	0.111	0.014
Topoisomerase II inhibitor	0.525	0.049
Tumour necrosis factor antagonist	0.180	0.145
Tyrosine kinase inhibitor	0.159	0.122
Urokinase inhibitor	0.340	0.107
Vitamin	0.249	0.181

Enhanced NCI database browser 2.1

Operations with this Structure (NSC 619198):

Structure
Retrieval:Format:

Fields:

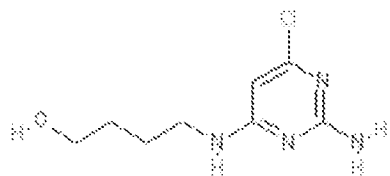
Cell Screens:

GI50 Screen

Visualization:

Format:

Structure Data:



NSC Number: 619198 Date: 2011-09-07 05:01

File Record: 210851 CAS Number: (None)

Formula: C₈H₁₃ClN₄O Weight: 216.6699 gr/mol

Complexity: 160.3 Anti-HIV Screening: No data available

Druglikeness(std): Is drug logP(KOW): 0.16

Druglikeness(neg): Is drug logP(exp): No data

WDI Record: No logP(ACD): No data

H-Bond Acceptors: 5 Available on DTP Plates: Yes

H-Bond Donors: 3

Rotatable Bonds: (CACTVS) 5 WLN: No data

Stereochemistry Potential R/S atoms and E/Z bonds No Yeast Screen Level 1

Catalyst Conformers: 25 Matched Conformer: None
(0 if Catalyst could not handle structure)

Composition: C 44.35% H 6.05% N 25.86% Cl 16.36% O 7.38%

SMILES: NC1=NC(=CC(=N1)NCCCCO)Cl

Name: 4-((2-amino-6-chloro-4-pyrimidinyl)amino)-1-butanol (ACD/Name 4.0)

Commercial Availability: No

Commercial Database Keys: None

Available Screening Data: TGI, LC₅₀, GI₅₀, YeastAnti-HIV Screening: No data (EC₅₀/IC₅₀) available.

Cancer Screening Summary:	Cell	log(Concentration)	-log(GI ₅₀)	-log(TGI)	-log(LC ₅₀)
	NCI-H23	-4.00m	4.000	4.000	4.000
	A549/ATCC	-4.00m	4.000	4.000	4.000
	EKVX	-4.00m	4.000	4.000	4.000
	NCI-H226	-4.00m	4.000	4.000	4.000
	NCI-H322M	-4.00m	4.000	4.000	4.000
	NCI-H460	-4.00m	4.000	4.000	4.000
	HOP-18	-4.00m	4.000	4.000	4.000
	HOP-92	-4.00m	4.000	4.000	4.000
	LXFL 529	-4.00m	4.000	4.000	4.000
	DMS 114	-4.00m	4.000	4.000	4.000
	DMS 273	-4.00m	4.000	4.000	4.000
	HT29	-4.00m	4.000	4.000	4.000
	HCC-2998	-4.00m	4.000	4.000	4.000
	HCT-116	-4.00m	4.000	4.000	4.000
	SW-620	-4.00m	4.000	4.000	4.000
	COLO 205	-4.00m	4.000	4.000	4.000
	DLD-1	-4.00m	4.000	4.000	4.000

HCT-15	-4.00m	4.000	4.000	4.000
KM12	-4.00m	4.000	4.000	4.000
KM20L2	-4.00m	4.000	4.000	4.000
OVCAR-4	-4.00m	4.000	4.000	4.000
OVCAR-5	-4.00m	4.000	4.000	4.000
OVCAR-8	-4.00m	4.000	4.000	4.000
IGR-OV1	-4.00m	4.000	4.000	4.000
SK-OV-3	-4.00m	4.000	4.000	4.000
CCRF-CEM	-4.00m	4.000	4.000	4.000
K-562	-4.00m	4.000	4.000	4.000
MOLT-4	-4.00m	4.000	4.000	4.000
HL-60(TB)	-4.00m	4.000	4.000	4.000
RPMI-8226	-4.00m	4.000	4.000	4.000
SR	-4.00m	4.000	4.000	4.000
UO-31	-4.00m	4.000	4.000	4.000
SN12C	-4.00m	4.000	4.000	4.000
A498	-4.00m	4.000	4.000	4.000
RXF-393	-4.00m	4.000	4.000	4.000
RXF-631	-4.00m	4.000	4.000	4.000
ACHN	-4.00m	4.000	4.000	4.000
TK-10	-4.00m	4.000	4.000	4.000
LOX IMVI	-4.00m	4.000	4.000	4.000
MALME-3M	-4.00m	4.000	4.000	4.000
SK-MEL-2	-4.00m	4.000	4.000	4.000
SK-MEL-5	-4.00m	4.000	4.000	4.000
SK-MEL-28	-4.00m	4.000	4.000	4.000
M19-MEL	-4.00m	4.000	4.000	4.000
UACC-62	-4.00m	4.000	4.000	4.000
UACC-257	-4.00m	4.000	4.000	4.000
SNB-19	-4.00m	4.000	4.000	4.000
SNB-75	-4.00m	4.185	4.000	4.000
SNB-78	-4.00m	4.798	4.000	4.000
U251	-4.00m	4.000	4.000	4.000
SF-268	-4.00m	4.000	4.000	4.000
SF-295	-4.00m	4.000	4.000	4.000
SF-539	-4.00m	4.000	4.000	4.000
XF 498	-4.00m	4.000	4.000	4.000

PASS Predictions:

Predicted Activity	p(active)	p(inactive)
Acetylcholine agonist	0.224	0.061
Acetylcholine muscarinic agonist	0.117	0.109
Acetylcholine nicotinic agonist	0.282	0.050
Adenosine A2a receptor agonist	0.183	0.030
Adenosine A2a receptor antagonist	0.065	0.047
Adenosine A2 receptor agonist	0.031	0.020
Adenosine deaminase inhibitor	0.044	0.036
Antibiotic Trimethoprim-like	0.112	0.006
Antihypercholesterolemic	0.293	0.113
Antiinfective (HIV)	0.549	0.021
Antimalarial	0.306	0.029
Antimetabolite	0.247	0.018
Antineoplastic	0.283	0.157
Antiobesity	0.274	0.079
Antiosteoporotic	0.224	0.154
Antiprotozoal	0.387	0.035
Antismoking	0.495	0.019
Antitrichomonal	0.311	0.045
Antitrypanosomal	0.338	0.033
Antiviral	0.673	0.010
Antiviral (HIV)	0.426	0.017
Antiviral (influenza)	0.109	0.002
Atherosclerosis treatment	0.636	0.058
Benzodiazepine agonist partial	0.181	0.064
Bone formation stimulant	0.278	0.197
Carcinogenic	0.158	0.130
Cholinergic agonist	0.310	0.174
Cytostatic	0.375	0.055

Dihydrofolate reductase inhibitor	0.126	0.006
Diuretic	0.228	0.147
Erythropoietin	0.453	0.027
Factor VIIa inhibitor	0.284	0.219
Geranylgeranyltransferase inhibitor	0.326	0.289
Glycinamide ribonucleotide formyltransferase inhibitor	0.048	0.017
Growth stimulant	0.166	0.148
Hair growth promoter	0.191	0.058
HDL-cholesterol increasing	0.299	0.131
Hematopoietic inhibitor	0.459	0.014
3 Hydroxyanthranilate oxygenase inhibitor	0.295	0.155
5 Hydroxytryptamine 3 agonist	0.546	0.014
Hypnotic	0.360	0.308
Interferon inducer	0.275	0.054
Interleukin 6 antagonist	0.362	0.272
Interleukin 8 antagonist	0.162	0.091
Maillard reaction inhibitor	0.161	0.136
Multiple sclerosis treatment	0.642	0.043
Muscle relaxant	0.218	0.177
Myocardial ischemia treatment	0.352	0.219
Neuropeptide antagonist	0.360	0.067
Neuropeptide Y antagonist	0.360	0.067
Nucleotide metabolism regulator	0.311	0.220
O6-alkylguanine-DNA alkyltransferase inhibitor	0.101	0.010
Phospholipase C inhibitor	0.485	0.087
Protein kinase C inhibitor	0.237	0.066
Purine nucleoside phosphorylase inhibitor	0.061	0.024
Purinergic P2 antagonist	0.159	0.023
Purinergic P2T antagonist	0.109	0.019
Purinergic receptor antagonist	0.159	0.023
Radiosensitizer	0.249	0.146
Respiratory distress syndrome treatment	0.333	0.290
Reverse transcriptase inhibitor	0.425	0.009
Saluretic	0.159	0.151
Septic shock treatment	0.448	0.059
Skeletal muscle relaxant	0.220	0.175
Sodium channel blocker	0.428	0.046
Teratogen	0.229	0.166
Teratogen and/or embryotoxic	0.229	0.166
Thymidine kinase inhibitor	0.319	0.068
Thymidylate synthase inhibitor	0.095	0.020
Topoisomerase II inhibitor	0.382	0.236
Tumour necrosis factor antagonist	0.214	0.078
Urokinase inhibitor	0.323	0.128

Enhanced NCI database browser 2.1

Operations with this Structure (NSC 636346):

Structure
Retrieval:Format:

Fields:

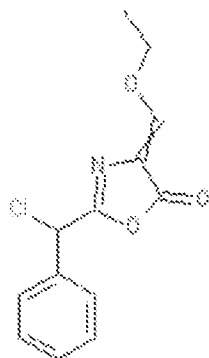
Cell Screens:

GI50 Screen Format:

Visualization:

Format:

Structure Data:



NSC Number: 636346 Date: 2011-09-07 04:58

File Record: 219796 CAS Number: (None)

Formula: C₁₃H₁₂ClNO₃ Weight: 265.6957 gr/mol

Complexity: 345.1 Anti-HIV Screening: Confirmed inactive

Druglikeness(std): No drug logP(KOW): 2.18

Druglikeness(neg): No drug logP(exp): No data

WDI Record: No logP(ACD): No data

H-Bond Acceptors: 4 Available on DTP Plates: Yes

H-Bond Donors: 0

Rotatable Bonds: (CACTVS) 4 WLN: No data

Stereochemistry Potential R/S atoms and E/Z bonds Yes

Yeast Screen Level 0

Catalyst Conformers: 8
(0 if Catalyst could not handle structure)

Matched Conformer: None

Composition: C 58.77% H 4.55% N 5.27% Cl 13.34% O 18.07%

SMILES: CCOC=C1N=C(OC1=O)C(Cl)C2=CC=CC=C2

Name: 2-(chloro(phenyl)methyl)-4-(ethoxymethylene)-1,3-oxazol-5(4H)-one (ACD/Name 4.0)

Commercial Availability: No

Commercial Database Keys: None

Available Screening Data: TGI, LC₅₀, GI₅₀, EC₅₀, IC₅₀

Anti-HIV Screening: Conclusion: Confirmed Inactive

IC₅₀(0.0001m) > 0.0001EC₅₀(0.0001m) > 0.0001

Cancer Screening Summary:

Cell	log(Concentration)	-log(GI ₅₀)	-log(TGI)	-log(LC ₅₀)
NCI-H23	-4.00m	4.000	4.000	4.000
NCI-H522	-4.00m	4.000	4.000	4.000
A549/ATCC	-4.00m	4.000	4.000	4.000
EKVX	-4.00m	4.000	4.000	4.000
NCI-H226	-4.00m	4.000	4.000	4.000
NCI-H322M	-4.00m	4.000	4.000	4.000
NCI-H460	-4.00m	4.000	4.000	4.000
HOP-62	-4.00m	4.000	4.000	4.000

HOP-92	-4.00m	4.000	4.000	4.000
LXFL 529	-4.00m	4.000	4.000	4.000
DMS 114	-4.00m	4.211	4.000	4.000
DMS 273	-4.00m	4.000	4.000	4.000
HT29	-4.00m	4.000	4.000	4.000
HCC-2998	-4.00m	4.000	4.000	4.000
SW-620	-4.00m	4.000	4.000	4.000
COLO 205	-4.00m	4.000	4.000	4.000
DLD-1	-4.00m	4.000	4.000	4.000
HCT-15	-4.00m	4.000	4.000	4.000
KM12	-4.00m	4.000	4.000	4.000
KM20L2	-4.00m	4.000	4.000	4.000
OVCAR-3	-4.00m	4.000	4.000	4.000
OVCAR-4	-4.00m	4.000	4.000	4.000
OVCAR-5	-4.00m	4.000	4.000	4.000
OVCAR-8	-4.00m	4.000	4.000	4.000
IGR-OV1	-4.00m	4.000	4.000	4.000
CCRF-CEM	-4.00m	4.000	4.000	4.000
K-562	-4.00m	4.000	4.000	4.000
MOLT-4	-4.00m	4.000	4.000	4.000
HL-60(TB)	-4.00m	4.000	4.000	4.000
RPMI-8226	-4.00m	4.000	4.000	4.000
UO-31	-4.00m	4.000	4.000	4.000
SN12C	-4.00m	4.000	4.000	4.000
A498	-4.00m	4.000	4.000	4.000
CAKI-1	-4.00m	4.000	4.000	4.000
RXF-393	-4.00m	4.000	4.000	4.000
786-0	-4.00m	4.000	4.000	4.000
ACHN	-4.00m	4.000	4.000	4.000
TK-10	-4.00m	4.000	4.000	4.000
LOX IMVI	-4.00m	4.000	4.000	4.000
MALME-3M	-4.00m	4.000	4.000	4.000
SK-MEL-2	-4.00m	4.000	4.000	4.000
SK-MEL-5	-4.00m	4.000	4.000	4.000
SK-MEL-28	-4.00m	4.000	4.000	4.000
M14	-4.00m	4.000	4.000	4.000
M19-MEL	-4.00m	4.000	4.000	4.000
UACC-62	-4.00m	4.000	4.000	4.000
UACC-257	-4.00m	4.000	4.000	4.000
SNB-19	-4.00m	4.000	4.000	4.000
SNB-75	-4.00m	4.000	4.000	4.000
SNB-78	-4.00m	4.000	4.000	4.000
SF-268	-4.00m	4.000	4.000	4.000
SF-295	-4.00m	4.000	4.000	4.000
SF-539	-4.00m	4.000	4.000	4.000
XF 498	-4.00m	4.000	4.000	4.000
SK-OV-3	-4.00m	(No data)	(No data)	(No data)

PASS Predictions:

Predicted Activity	p(active)	p(inactive)
Acetylcholine agonist	0.193	0.091
Acetylcholine antagonist	0.154	0.148
Acetylcholine M1 receptor agonist	0.096	0.070
Acetylcholine M2 receptor antagonist	0.173	0.143
Acetylcholine M3 receptor antagonist	0.202	0.100
Acetylcholine muscarinic agonist	0.131	0.075
Acetylcholine muscarinic antagonist	0.173	0.125
Acetylcholine nicotinic agonist	0.281	0.051
Acetylcholine nicotinic antagonist	0.181	0.092
Acetylcholine release stimulant	0.373	0.045
Acute neurologic disorders treatment	0.231	0.221
Adenosine A2a receptor antagonist	0.062	0.057
Adenosine A3 receptor antagonist	0.337	0.086
Adenosine kinase inhibitor	0.111	0.110

ADP ribosyl transferase inhibitor	0.306	0.026
Adrenergic transmitter uptake inhibitor	0.415	0.104
Alcohol dehydrogenase inhibitor	0.300	0.048
Aldosterone antagonist	0.198	0.067
Alkylator	0.106	0.078
Alkylphospholipid	0.074	0.053
Alpha 1 adrenoreceptor agonist	0.285	0.055
Alpha 2 adrenoreceptor agonist	0.149	0.059
Alpha adrenoreceptor agonist	0.130	0.072
Alpha glucosidase inhibitor	0.065	0.065
Alzheimer's disease treatment	0.434	0.057
Aminopeptidase microsomal inhibitor	0.329	0.086
AMPA receptor agonist	0.120	0.043
Anabolic	0.160	0.063
Analeptic	0.383	0.047
Androgen agonist	0.077	0.058
Anesthetic	0.200	0.122
Anesthetic general	0.251	0.067
Anesthetic inhalation	0.374	0.012
Anesthetic local	0.196	0.120
Angiogenesis inhibitor	0.275	0.215
Anorexic	0.336	0.048
Antiamoebic	0.303	0.069
Antiasthmatic	0.313	0.183
Anticataract	0.290	0.079
Anticerebroischemic	0.320	0.169
Anticoccidial	0.190	0.107
Anticonvulsant	0.248	0.186
Antidepressant, Imipramin-like	0.187	0.090
Antidiabetic	0.211	0.134
Antidiabetic symptomatic	0.171	0.124
Antidyskinetic	0.457	0.093
Antiemphysemic	0.122	0.111
Antifungal	0.228	0.167
Antiglaucomic	0.188	0.148
Anti-Helicobacter pylori	0.220	0.131
Antihelminthic	0.300	0.066
Antihypercholesterolemic	0.395	0.057
Antiinfective (HIV)	0.326	0.164
Antiinflammatory, intestinal	0.391	0.146
Antiinflammatory, pancreatic	0.341	0.152
Antiischemic	0.409	0.213
Antilipidemic	0.357	0.070
Antimalarial	0.190	0.128
Antimycobacterial	0.248	0.108
Antineoplastic	0.348	0.118
Antineoplastic enhancer	0.329	0.073
Antioxidant	0.191	0.119
Antiparkinsonian, rigidity relieving	0.355	0.064
Antiparkinsonian, tremor relieving	0.294	0.078
Antipruritic	0.514	0.069
Antipsoriatic	0.256	0.189
Antiseptic	0.586	0.018
Antismoking	0.353	0.078
Antispirochetal	0.191	0.086
Antitoxic	0.376	0.063
Antitrichomonal	0.283	0.061
Antitrypanosomal	0.276	0.081
Antitussive	0.229	0.108
Antitussive, narcotic	0.197	0.086
Antiulcerative	0.261	0.182
Antiviral	0.306	0.109

Antiviral (hepatitis)	0.428	0.031
Antiviral (hepatitis C)	0.337	0.034
Arrhythmogenic	0.562	0.106
Atherosclerosis treatment	0.443	0.193
Benzodiazepine agonist partial	0.153	0.109
Benzodiazepine antagonist	0.199	0.069
Benzodiazepine inverse agonist	0.089	0.056
Beta 1 adrenoceptor agonist	0.101	0.094
Beta lactamase inhibitor	0.072	0.062
Bone formation stimulant	0.400	0.088
Bone resorption inhibitor	0.329	0.114
Calcium regulator	0.286	0.102
Calmodulin antagonist	0.217	0.130
Calpain inhibitor	0.189	0.069
cAMP phosphodiesterase inhibitor	0.339	0.138
Cannabinoid receptor agonist	0.236	0.077
Carcinogenic	0.369	0.037
Cardiodepressant	0.303	0.151
Cardioprotectant	0.348	0.085
Cardiotoxic	0.337	0.072
Cardiovascular analeptic	0.691	0.029
Catechol O methyltransferase inhibitor	0.265	0.067
Cathepsin B inhibitor	0.136	0.128
Cathepsin L inhibitor	0.298	0.048
Chemopreventive	0.556	0.048
Choleretic	0.261	0.076
Cholesterol esterase inhibitor	0.141	0.042
Cholinergic agonist	0.398	0.071
Cholinergic antagonist	0.135	0.084
CNS active muscle relaxant	0.383	0.065
Coagulant	0.171	0.037
Cocain dependency treatment	0.340	0.063
Complement inhibitor	0.394	0.206
Contraceptive	0.235	0.100
Corneal wound healing stimulator	0.285	0.222
Cyclooxygenase inhibitor	0.207	0.125
Cystic fibrosis treatment	0.330	0.106
Cytokine modulator	0.427	0.163
Cytosole dipeptidase inhibitor	0.321	0.090
Cytostatic	0.330	0.079
Dihydroorotate dehydrogenase inhibitor	0.214	0.044
Dipeptidyl aminopeptidase IV inhibitor	0.171	0.067
Diuretic	0.233	0.136
Dopa decarboxylase inhibitor	0.309	0.048
Dopamine beta hydroxylase inhibitor	0.086	0.043
Dopamine uptake inhibitor	0.143	0.107
Embryotoxic	0.429	0.047
Endothelin antagonist	0.261	0.098
Erythropoietin	0.396	0.064
Estrone sulfatase inhibitor	0.144	0.101
Excitatory amino acid agonist	0.278	0.034
Excitatory amino acid antagonist	0.288	0.089
Expectorant	0.277	0.061
Factor XIIIa inhibitor	0.103	0.097
GABA aminotransferase inhibitor	0.149	0.056
GABA A receptor agonist	0.246	0.109
GABA A receptor antagonist	0.161	0.075
GABA B receptor agonist	0.218	0.041
GABA B receptor antagonist	0.127	0.042
GABA receptor agonist	0.361	0.072
GABA receptor antagonist	0.284	0.042
GABA uptake inhibitor	0.130	0.097

Geranylgeranyltransferase inhibitor	0.349	0.168
Glucagon receptor antagonist	0.255	0.126
Glucose-6-phosphate translocase inhibitor	0.179	0.085
Glutamate (mGluR1a) agonist	0.119	0.030
Glutamate (mGluR1) agonist	0.094	0.034
Glutamate (mGluR1) antagonist	0.071	0.037
Glutamate (mGluR2) agonist	0.149	0.029
Glutamate (mGluR2) antagonist	0.115	0.043
Glutamate (mGluR3) agonist	0.120	0.034
Glutamate (mGluR3) antagonist	0.154	0.047
Glutamate (mGluR5a) agonist	0.119	0.030
Glutamate (mGluR5) agonist	0.192	0.031
Glutamate (mGluR5) antagonist	0.421	0.027
Glutamate (mGluR6) agonist	0.072	0.045
Glutamate (mGluR6) antagonist	0.159	0.039
Glutamate (mGluR) agonist	0.048	0.038
Glutamate (mGluR) antagonist	0.163	0.041
Glutamate receptor agonist	0.083	0.049
Glutamate uptake inhibitor	0.137	0.042
Glycine receptor agonist	0.288	0.028
Gynecological disorders treatment	0.214	0.180
Hair growth promoter	0.156	0.113
HCV NS3-helicase inhibitor	0.162	0.039
HCV NS3 protease inhibitor	0.340	0.167
HCV serine protease inhibitor	0.231	0.163
HDL-cholesterol increasing	0.436	0.056
Hematopoietic	0.180	0.134
Hematopoietic inhibitor	0.381	0.033
Hepatoprotectant	0.320	0.070
Hestagen antagonist	0.345	0.071
Histamine agonist	0.072	0.044
Histamine H1 receptor antagonist	0.239	0.096
Histamine H2 receptor agonist	0.210	0.051
Histamine H3 receptor agonist	0.071	0.033
Histamine release stimulant	0.442	0.085
Histidine decarboxylase inhibitor	0.110	0.056
HIV integrase inhibitor	0.384	0.087
HMG CoA synthase inhibitor	0.101	0.080
3 Hydroxyanthranilate oxygenase inhibitor	0.319	0.051
5 Hydroxytryptamine 2 agonist	0.342	0.088
5 Hydroxytryptamine 2B antagonist	0.158	0.155
5 Hydroxytryptamine 2C agonist	0.392	0.079
5 Hydroxytryptamine 3 agonist	0.307	0.061
5 Hydroxytryptamine release stimulant	0.389	0.070
Hypertensive	0.339	0.075
Hypertensive, ophthalmic	0.271	0.051
Hypertermic	0.270	0.068
Hypnotic	0.529	0.041
Hypoglycemic	0.181	0.096
Hypotermic	0.443	0.110
Ileal bile acid transport inhibitor	0.150	0.141
Immunostimulant	0.234	0.225
Immunosuppressant	0.247	0.237
Insulin promoter	0.355	0.122
Insulin secretagogues	0.158	0.070
Interferon inducer	0.246	0.098
Interleukin 1 antagonist	0.331	0.170
Interleukin 6 antagonist	0.415	0.105
Interleukin 8 antagonist	0.151	0.143
Interleukin antagonist	0.284	0.195
Kainate receptor agonist	0.111	0.056
Kainate receptor antagonist	0.123	0.087

Keratolytic	0.493	0.076
Keratoses actinic(solar) treatment	0.352	0.068
Leukopoiesis inhibitor	0.428	0.045
Lipid peroxidase inhibitor	0.219	0.163
Liver fibrosis treatment	0.232	0.085
Lymphocytopoiesis inhibitor	0.175	0.070
Maillard reaction inhibitor	0.208	0.055
Male reproductive disfunction treatment	0.398	0.177
Mannosidase inhibitor	0.214	0.031
MAO-A inhibitor	0.170	0.066
MAO-B inhibitor	0.098	0.068
MAO inhibitor	0.247	0.082
Mediator release inhibitor	0.285	0.156
Melatonin antagonist	0.344	0.067
Metabolic	0.565	0.105
Miotic	0.314	0.047
Mucolytic	0.198	0.062
Multiple sclerosis treatment	0.393	0.248
Muscle relaxant	0.290	0.106
Mutagenic	0.237	0.041
Mydriatic	0.126	0.074
Myocardial ischemia treatment	0.386	0.175
Narcotic antagonist	0.228	0.131
Nasal decongestant	0.253	0.061
Neurotrophic factor	0.368	0.210
Nitric oxide donor	0.052	0.045
Nitric oxide synthase inhibitor	0.197	0.053
NMDA receptor agonist	0.185	0.038
NMDA receptor antagonist	0.106	0.095
NMDA receptor glycine site agonist	0.461	0.021
NMDA receptor glycine site antagonist	0.112	0.040
NMDA receptor polyamine site activator	0.209	0.022
NMDA receptor polyamine site blocker	0.068	0.061
Non-steroidal antiinflammatory agent	0.303	0.065
Nootropic	0.469	0.058
Nucleotide metabolism regulator	0.464	0.100
O6-alkylguanine-DNA alkyltransferase inhibitor	0.064	0.040
Ophthalmic drug	0.243	0.156
Opioid antagonist	0.135	0.118
Opioid partial agonist	0.179	0.167
Ornithine decarboxylase inhibitor	0.137	0.039
2,3-Oxidosqualene-lanosterol cyclase inhibitor	0.237	0.103
Oxytocin agonist	0.226	0.173
Parathyroid hormone antagonist	0.255	0.136
Phosphodiesterase I inhibitor	0.176	0.109
Phosphodiesterase V Inhibitor	0.195	0.189
Phospholipase C inhibitor	0.453	0.124
Photosensitizer	0.114	0.082
Platelet adhesion inhibitor	0.397	0.054
Platelet antagonist	0.282	0.071
Poly(ADP-ribose)synthetase inhibitor	0.340	0.060
Postcoital contraceptive	0.138	0.120
Progestin agonist	0.130	0.076
Prolactin inhibitor	0.252	0.094
Prolyl endopeptidase inhibitor	0.058	0.056
Prostaglandin antagonist	0.274	0.102
Protease inhibitor	0.150	0.148
Protocollagen prolyl hydroxylase inhibitor	0.088	0.056
Psychosexual dysfunction treatment	0.397	0.151
Psychostimulant	0.445	0.053
Quisqualate antagonist	0.124	0.043
Radioprotector	0.383	0.050

Radiosensitizer	0.295	0.087
Respiratory analeptic	0.407	0.048
Respiratory distress syndrome treatment	0.367	0.242
Reverse transcriptase inhibitor	0.158	0.112
Rhinitis treatment	0.312	0.295
Ribonucleotide reductase inhibitor	0.140	0.132
S-adenosyl-L-methionine decarboxylase inhibitor	0.318	0.034
Saluretic	0.190	0.066
Saluretic, reabsorption inhibitor	0.129	0.068
Sclerosant	0.292	0.039
Sedative	0.322	0.140
Skeletal muscle relaxant	0.291	0.097
Sodium channel blocker	0.389	0.078
Sodium channel blocker class Ib	0.318	0.036
Spasmogenic	0.308	0.116
Spasmolytic	0.213	0.213
Spasmolytic, Papaverin-like	0.264	0.112
Spasmolytic, urinary	0.264	0.177
Spermicide	0.592	0.053
Squalene epoxidase inhibitor	0.161	0.080
Succinic dehydrogenase inhibitor	0.150	0.044
Sympatholytic	0.350	0.083
Teratogen	0.410	0.048
Teratogen and/or embryotoxic	0.410	0.048
Thrombolytic	0.274	0.102
Thymidine kinase inhibitor	0.312	0.086
Thyroid hormone agonist	0.113	0.070
Thyroid hormone antagonist	0.169	0.034
TNF-alpha release inhibitor	0.488	0.091
Topoisomerase II inhibitor	0.450	0.105
Tyrosine kinase inhibitor	0.148	0.141
Ulcerogenic	0.282	0.064
Uricosuric	0.432	0.078
Uridine phosphorylase inhibitor	0.112	0.058
Urokinase inhibitor	0.320	0.135
Vasodilator	0.223	0.222
Vasopressor	0.294	0.232
Vitamin	0.268	0.120
Xanthine oxidase inhibitor	0.251	0.084

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